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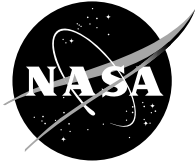
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Abstract

Solid oxide fuel cell systems used in the aerospace or commercial aviation environment require a compact, light-weight and highly durable catalytic fuel processor. The fuel processing method considered here is an autothermal reforming (ATR) step. The ATR converts Jet-A fuel by a reaction with steam and air forming hydrogen (H_2) and carbon monoxide (CO) to be used for production of electrical power in the fuel cell. This paper addresses the first phase of an experimental catalyst screening study, looking at the relative effectiveness of several monolith catalyst types when operating with untreated Jet-A fuel. Six monolith catalyst materials were selected for preliminary evaluation and experimental bench-scale screening in a small 0.05 kW_e micro-reactor test apparatus. These tests were conducted to assess relative catalyst performance under atmospheric pressure ATR conditions and processing Jet-A fuel at a steam-to-carbon ratio of 3.5, a value higher than anticipated to be run in an optimized system. The average reformer efficiencies for the six catalysts tested ranged from 75 to 83 percent at a constant gas-hourly space velocity of 12,000 hr⁻¹. The corresponding hydrocarbon conversion efficiency varied from 86 to 95 percent during experiments run at reaction temperatures between 750 to 830 °C. Based on the results of the short-duration 100 hr tests reported herein, two of the highest performing catalysts were selected for further evaluation in a follow-on 1000 hr life durability study in Phase II.

1. Introduction

Solid oxide fuel cell (SOFC) systems are being studied by the NASA Glenn Research Center (Glenn) (ref. 1) for commercial aerospace and general aviation application. These applications include on-board generation of auxiliary power or propulsive thrust. The aviation platforms include unmanned aerial vehicles (fig. 1) and commercial air transportation systems. An aviation fuel cell based system that utilizes Jet-A fuel as the feed is preferred as it can be readily integrated within the existing aircraft infrastructure. The on-board reformer must have the ability to convert the liquid Jet-A hydrocarbon into a synthesis gas (reformat) that's rich in hydrogen (H_2) and carbon monoxide (CO). This reformat then feeds directly into the solid oxide fuel cell stack where power and waste heat are produced. The reformer reactor technology, necessary for on-board deployment with aircraft, must have features including compactness, light weight and high durability. Monolithic catalysts offer high surface area to volume



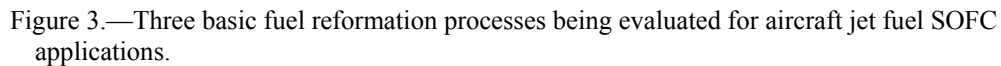
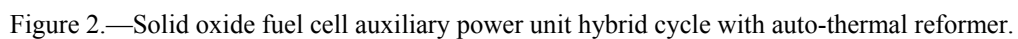
Figure 1.—The Helios prototype unmanned aerial vehicle on approach for a dry lake-bed landing.

ratios, are known to have high relative activity, are durable at extreme temperature, their resistant to vibrational affects and produce very low pressure drop (ref. 2).

An in-house fuel processing program that's been ongoing at Glenn has the objective to develop a reformer technology that meets the stringent requirements of commercial solid oxide fuel cell based air transportation power systems. This paper describes the results of a series of catalyst screening tests conducted with Jet-A fuel under autothermal reforming (ATR) process conditions. The experimental testing portion of the Phase I work was contracted to the SOFCo-EFS Holdings, LLC, by Glenn and funded under the former Low Emission Alternate Power (LEAP) program. The combined NASA-SOFCo team has extensive experience with distillate fuels, fuel processing technology, and the integration of hybrid fuel cell power systems. One particular goal of the program is to develop a viable reforming approach for Jet-A fuel that provides a suitable fuel gas for use with solid oxide fuel cells (SOFC), while yielding compact, light weight, high efficiency and cost-effective hybrid auxiliary power units (APU), an example of which is shown in figure 2.

NASA Glenn is also investigating advanced direct fuel injection methods for reformer reactors (ref. 3) in addition to Jet fuel and reformat desulfurization technologies. Since all of the system trade studies for aircraft APU are still in-progress, Glenn will evaluate all three basic catalytic reformer processes represented in figure 3. These potential technologies include steam reforming (SR), catalytic partial oxidation (CPOX) and, autothermal reforming (ATR).

The ATR monolith catalytic process using untreated, sulfur containing Jet-A fuel is the topic of this paper. The work described in this report and, briefly summarized elsewhere (ref. 4), is focused on the evaluation of six monolith catalysts tested under auto-thermal reforming conditions with straight-run, untreated Jet-A fuel containing 1,500 ppm_w sulfur. These evaluations consisted of short-duration, 70 to 100 hr tests at constant reactor operating conditions. Steam-to-carbon (S:C) and atomic oxygen-to-carbon (O:C) feed ratios were maintained fixed at 3.51 and 0.72, respectively. Experiments were conducted at a constant gas hourly space velocity of 12,000 hr⁻¹ over a reactor temperature range from 750 to 830 °C. The ATR catalyst screening tests were carried out at the SOFCo-EFS test facility in July through August, 2003.



<i>ATR</i>	autothermal reforming
<i>C-Bal</i>	carbon molar balance experimental, (percent)
<i>F</i>	molar flow rate, (g-mol/hr)
<i>GHSV</i>	gas hourly space velocity, (hr ⁻¹) @ 0.0 °C, 760 mm Hg

$LHSV$	liquid hourly space velocity, (hr^{-1})
LHV	lower heating value, (kJ/g or kJ/g-mol)
MW	molecular weight, (g/g-mol)
n_i	moles of carbon per mole of species “ i ”
N_j	moles of species “ j ” per mole of fuel
$N\text{-}Bal$	nitrogen molar balance experimental, (percent)
$O:C$	oxygen : carbon molar feed ratio, ($\text{g-mol O} / \text{g-mol C}$)
P	pressure, (psia or atm)
Q	volumetric flow rate, (cm^3/hr or sccm)
R_g	ideal gas law constant, ($82.057 \text{ cm}^3 \cdot \text{atm/K} \cdot \text{g-mol}$)
$S:C$	steam : carbon molar feed ratio, ($\text{g-mol H}_2\text{O} / \text{g-mol C}$)
T	temperature, ($^{\circ}\text{C}$)
TOS	time-on-stream, (hr)
V	volume, (cm^3)
W	mass flow rate, (gm/hr)
x	mass fraction, (d-less)
y	mole fraction, (d-less)

Greek

ε	void fraction, (d-less)
η	thermal efficiency, (perc)
ϕ	equivalence ratio, (d-less)
ρ	density or specific gravity, gm/cm^3
θ	contact residence time, (s)
X	conversion efficiency, (percent)
Ω_{GC}	gas chromatograph correction factor to normalize raw data, $\Omega_{GC} = 0.970$

Subscripts/Superscripts

A	air
avg	average
b	bulk
C	carbon
cat	catalyst
F	fuel
f_{sp}	furnace set-point
HC	hydrocarbon
H_2	hydrogen
i	$\text{CO}, \text{CO}_2, \text{CH}_4, \text{C}_2\text{H}_4, \text{C}_2\text{H}_6, \dots \text{C}_n\text{H}_{2n}, \text{C}_n\text{H}_{2n+2}$
j	C, H, O, and S atoms
N_2	nitrogen
R	reformatte effluent
Ref	reformer
S	steam

3. Apparatus

The ATR monolith catalyst evaluations were carried out using a modified Zeton-Altamira AMI-200 unit shown in figure 4. The apparatus was equipped with a de-ionized (DI) water feed pump, a Jet fuel feed syringe pump, water and fuel vaporizers, a clam shell furnace and a condensate knockout trap. The



Figure 4.—Zeton-Altamira catalyst screening test rig.

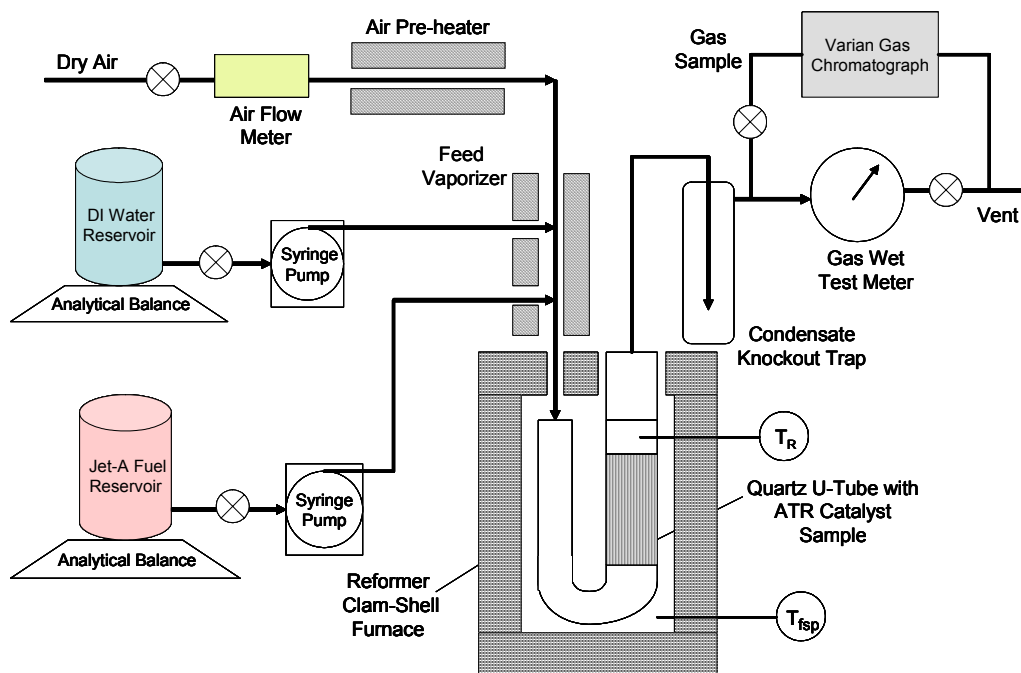


Figure 5.—Micro-reactor catalyst screening apparatus—test schematic.

micro-reactor was a U-shaped quartz glass tube. The left arm of the reactor was 0.25 in. OD and served to reheat the air-steam-fuel feed streams to the furnace set-point temperature (T_{fsp}) and the 0.75 in. OD right arm contained the fresh monolith catalyst sample.

The reactor operated at constant wall temperature, controlled by an external heater. It was also non-adiabatic, with heat loss normally directed from the catalyst bed towards the furnace. The effluent hot gas temperature (T_R) out of the quartz glass reactor was measured with a single Type K thermocouple. The reactor effluent gas was analyzed on-line using a Varian CP2003 Quad Micro-GC gas chromatograph calibrated with standard gaseous mixtures. The reactor product effluent flow rate (Q_R) was measured downstream of the condensate knockout trap using a wet test flow meter. A schematic of the micro-reactor catalyst screening test apparatus used in this experiment is shown in figure 5.

4. Test Procedures

Six bench-scale monolith catalyst screening experiments were conducted during the Phase I of the test protocol. The monolith catalyst was loaded inside the micro-reactor and wrapped with ceramic paper (Fiberfrax, Unifrax Corporation) which provided the gas seal between the monolith and quartz reactor wall. The U-tube reactor was placed in the furnace and preheated to 750 °C with hot air flowing through the system. Steam produced from DI water was then introduced and after the flow stabilized, the fuel syringe pump was started. After the steam, fuel and air flow rates were established, they were held constant through-out the entire screening run. The reactor effluent gas was analyzed on-line using a Varian CP2003 Quad Micro gas chromatograph (GC) calibrated with standard gaseous mixtures. The on-line results from the GC provided reformer effluent concentrations on a dry basis for H₂, CO, CO₂, CH₄, N₂, and the heavier C₂⁺ compounds.

The reactor effluent flow rate (Q_R) was measured downstream of the condensate knockout trap using a wet test flow meter. The testing protocol called for 50 to 100 hr of continuous micro-reactor operation. Data was taken periodically and at random time intervals during the course of the catalyst screening experiment. The shut-down procedure for the ATR micro-reactor was to stop fuel flow, then after approximately 30 min stop steam flow, and, lastly cool the reactor to room temperature with ambient air flowing through the reactor apparatus. At the completion of the test, the catalyst sample was removed and examined for signs of thermal sintering, degradation, monolith pore blockage, wear and/or carbon formation.

5. Experimental

5.1 Objectives

The objectives of the Phase I experimental ATR catalyst testing program were several fold. The first goal was to identify potential candidate monolith reformer catalysts for performance evaluation in a micro-reactor. These monolith catalysts would be screened under ATR conditions using un-treated (sulfur containing) Jet-A fuel. The screening would involve catalyst performance evaluation under short-term, standardized operating conditions in a 0.05 kW_e micro-reactor. The final objective in Phase I was to recommend one or more monolith catalyst systems for further evaluation and prolonged test in a Phase II 1000 hr life study.

5.2 Jet-A Fuel

The Jet-A fuel used for the testing was supplied to SOFCo by Glenn and identified as being Canton Terminal (Jet-A) from the BP Oil Company, Hartford Avenue, Canton, Ohio. Analytical test data (refs. 5 to 6) on the jet fuel used in these reformer tests is summarized in Table 1. The fuel characterization data provides Jet-A ultimate analysis, physical properties, trace metal content, distillation temperature cut-points and hydrocarbon type analysis. The fuel was subsequently reanalyzed for total sulfur by ASTM D-5453 and found to contain ~1500 ppm_w versus the 3100 ppm_w shown in the ultimate analysis results generated from ASTM D-129. This fuel therefore met all commercial Jet-A product specifications.

TABLE 1.—ANALYSIS OF JET-A FUEL
[PER ASTM 1655 (5–6)]

Description	Analysis	Remark/test method ASTM
Jet-A formula, average	$C_{11.5} \cdot H_{21.4}$	
Average molecular weight, g/g-mol	160.0	
Ultimate analysis		
Carbon, wt%	86.37	D3701
Hydrogen, wt%	13.48	
Sulfur, wt%	0.31	D129
H/C, wt%	0.157 to 0.158	
Total sulfur, ppm _w	1,488	D5453
Density, lb/ft ³	50.77	
Specific gravity, 60 °F	0.814	D71
API gravity, 60 °F	41.5	D287
Viscosity, 60 °F, cSt	1.863	D446
Lower heat of combustion, Btu/lb (kJ/g)	18,673 (43.435)	D4809
Trace metals		
Mg, ppm _w	0.57	E1479
Zn, ppm _w	0.58	
Al, ppm _w	0.23	
Cu, ppm _w	0.11	
Fe, ppm _w	0.34	
Ca, ppm _w	1.61	▼
Distillation		D86
10 percent Rec, °C	180	
50 percent Rec, °C	209	
90 percent Rec, °C	247	
FBP, °C	275	
Residue, vol%	1.0	▼
Flash point, °C	49	D56
Freeze point, °C	–57	D2386
Hydrocarbon type		D2789
Paraffins, vol%	36.5	
Monocycloparaffins, vol%	35.9	
Dicycloparaffins, vol%	12.8	
Alkylbenzenes, vol%	10.4	
Indans and Tetralins, vol%	3.3	
Naphthalenes, vol%	1.3	▼

5.3 Catalysts

Six developmental autothermal reforming catalysts in monolith form were obtained from several catalyst suppliers. The catalyst materials had cell densities in the range of 300 to 600 cores per square inch (cps) and bulk densities of 0.38 to 0.61 g/cc. The physical properties of these catalysts (ref. 7) used in the ATR tests are shown in table 2. The monolith test specimen dimensions used in the micro-reactor apparatus were all sized at 0.5 in. diameter and 3 in. long. The corresponding catalyst bed volume (V_{cat}) based on these monolith dimensions is 9.653 cm³ (0.589 in.³). Specific catalyst formulations in terms of base metal content, precious metal loading and/or substrate materials employed is unknown because that information is proprietary to each of the respective catalyst suppliers. Test results of specific catalyst material performance shall be reported through-out this paper with respect to generic catalyst formulation numbers designated A-2, B-6, C-5, D-3, E-1 and F-4. The numerical value preceding the primary letter of these identifiers indicates the catalysts' relative performance ranking based upon experimental test results.

TABLE 2.—ATR MONOLITH TEST SAMPLE CATALYST PROPERTIES (REF. 7)

Catalyst ID ¹	Bulk density, g/ml	Cell density, ² cpsi	Open frontal area, percent	Hydraulic ³ channel diameter, mm
A-2	0.51	400	82.8	1.156
B-6	0.38	400	82.8	1.156
C-5	0.55	400	82.8	1.156
D-3	0.56	300	62.9	1.168
E-1	0.61	600	83.0	0.947
F-4	0.49	600	83.0	0.947

¹All monolith catalyst sample sizes tested were 0.5 in. OD by 3.0 in. long.²Cell density has standard units of cores per square inch.³Hydraulic diameter for the monolith square channel cell shape is the opening width.

5.4 Bench-Scale Testing

The ATR catalyst screening test conditions are summarized in table 3. The micro-reactor monolith operating conditions that were held constant were: Jet-A fuel feed of 16.2 cm³/hr; deionized water feed rate of 60 cm³/hr; and, air feed rate of 600 sccm (dry). The standard testing protocol called for 50 to 100 hr of continuous ATR operation. During the run with catalyst sample B-6, testing was however, interrupted at 30 hr *TOS* due to a weekend shutdown. The experiment with sample E-1 was interrupted at 66 hr *TOS* due to a fuel pump stall. Otherwise, the remainder of the tests ran continuously and more or less unattended. The reactor effluent gas flow rate (Q_R) and reformat gas composition were periodically measured to determine the ATR catalyst performance. Also, the reactor furnace set-point temperature (T_{fsp}) was manually increased in an incremental fashion as necessary during screening tests in order to maintain a reformer efficiency (η_{Ref}) at a minimum value of approximately 70 percent. In other words, if the measured η_{Ref} started approaching or had dropped below 70 percent, the T_{fsp} was increased by a 20 °C increment.

TABLE 3.—MICRO-REACTOR ATR CATALYST SCREENING TEST CONDITIONS

Test parameter	Data symbol	Test condition
Pressure, psia	P_{Ref}	14.696
Furnace set temperature, °C	T_{fsp}	750 to 830
Jet-A feed rate, cm ³ /hr	Q_F	16.2
Deionized water feed rate, cm ³ /hr	Q_S	60
Air feed rate, sccm	Q_A	600
Steam-to-carbon feed ratio, mol H ₂ O/mol C	$S:C$	3.51
Oxygen-to-carbon feed ratio, mol O/mol C	$O:C$	0.72
Average gas hourly space velocity, hr ⁻¹	$GHSV_{avg}$	12,014
Average liquid hourly space velocity, hr ⁻¹	$LHSV_{avg}$	1.73
Equivalence ratio	ϕ	4.2
Contact time, sec ¹	θ	0.074 to 0.078

¹Feed gas flow rate at process conditions divided by the monolith bed volume.

Carbon and nitrogen mass balance variations estimated during the tests were in the 94 to 108 percent and 97 to 110 percent ranges, respectively. The latter were consistently higher suggesting some drift in air mass flow controller calibration. Since the nitrogen balances were consistent for all of the tests, the discrepancy should not affect the relative performance data. The exit gas temperature (T_R) from the monolith bed was monitored with a Type K thermocouple. Due to space limitations, the monolith exit was located nearer to the end of the furnace where the temperature gradient was high. Small changes in the position of the thermocouple relative to the monolith and the furnace affected the recorded bed exit temperature. Consequently, bed exit temperatures (T_R) are consistent within a given test run but T_R comparisons between various samples tested are less accurate. Figure 6 shows the spent but non-the-less

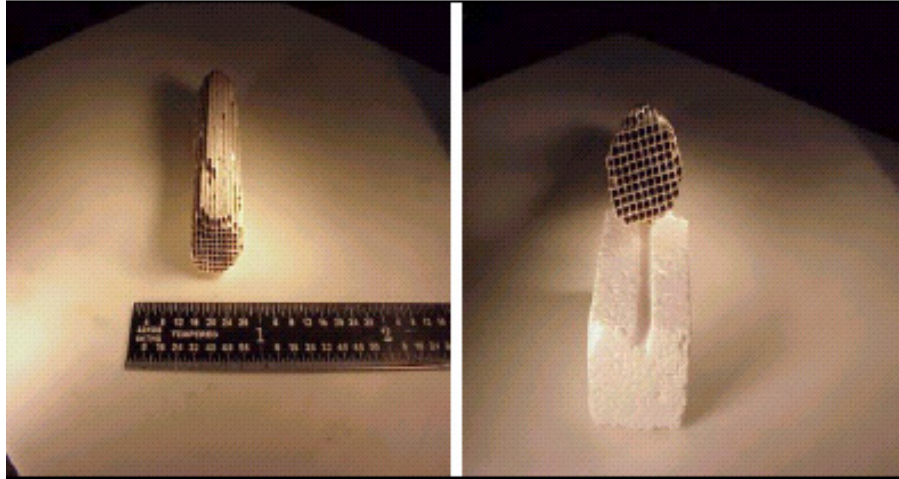


Figure 6.—Used ATR monolith catalyst sample E-1 after 90 hr TOS of test.

TABLE 4.—ATR CATALYST SCREENING TEST SUMMARY—AVERAGE PERFORMANCE DATA¹

Catalyst ID	Total TOS, hr	Furnace set pt. temp., °C	C-bal, percent	N-Bal, percent	HC conv., percent	Ref eff., percent	H ₂ conv. eff., percent	Reformate flow, dry basis (sccm)	Ranking Best = 1 Worst = 6
A-2	96.6	760	101	108	93	80	32	1328	2
B-6	100.9	789	102	109	86	75	25	1226	6
C-5	73.3	788	100	106	90	77	28	1256	5
D-3	67.3	770	99	105	92	78	27	1255	3
E-1	90.1	750	101	106	95	83	35	1383	1
F-4	102.8	777	99	108	92	77	30	1297	4

¹Reported values are time-averaged over the TOS test duration for each catalyst.

TABLE 5.—ATR CATALYST SCREENING SUMMARY—AVERAGE DRY REFORMATE GAS COMPOSITION¹

Catalyst ID	Dry reformate gas composition, mol %						Hydrogen and carbon monoxide, mol %
	H ₂	CH ₄	C ₂ ⁺	CO	CO ₂	N ₂	(H ₂ + CO)
A-2	36.8	1.1	0.37	13.0	11.2	37.5	49.8
B-6	31.8	1.6	1.04	18.1	6.6	40.8	49.9
C-5	34.2	1.5	0.59	16.1	8.6	39.0	50.3
D-3	33.6	1.5	0.39	17.9	7.5	39.2	51.5
E-1	39.4	1.0	0.16	11.0	13.0	35.4	50.4
F-4	34.8	1.4	0.33	13.7	10.2	38.1	48.5

¹Reported values are time-averaged over the TOS test duration for each catalyst.

intact ATR catalyst sample E-1 evaluated in the screening study after 90.1 hr TOS. Much like the E-1 sample, there was no visual evidence of carbon deposition, thermal sintering, pore blockage or any structural deterioration to any of the six monolith catalysts tested during the Phase I evaluation.

Table 4 summarizes the time-averaged performance test data obtained for the six monolith catalysts evaluated. Listed in table 5 are average reformate gas compositions based on the normalized GC measured data. The average reformer efficiencies for the catalysts ranged from 75 to 83 percent, while average hydrocarbon conversion was 86 to 95 percent. The time-averaged hydrogen conversion efficiency varied from 25 to 35 percent while average carbon balances were all approximately 100 percent. The reformate gas contained an average H₂ product concentration of 32 to 39 percent (dry-basis), a total hydrocarbon slippage ranging from 1.2 to 2.6 percent CH₄ + C₂⁺ and a mean H₂ + CO that was approximately 50 percent for all samples tested. The complete catalyst evaluation screening data set for each of the six monolith samples tested is found detailed in appendix A.

6. Data Reduction and Analysis

The various process parameters and calculations used to define and analyze the ATR catalyst performance data are presented in this section of the report.

6.1 Molar Feed Rates

The molar flow rates (g-mol/hr) for each of the respective micro-reactor feed streams, including Jet-A fuel (F_F), air (F_A), steam (F_S) and also, the carbon present in the fuel (F_C) feed are computed from the raw flow meter data with the following expressions.

$$F_F = \frac{Q_F \rho_F}{MW_F} \quad (1)$$

$$F_A = \frac{Q_A}{22,410} \quad (2)$$

$$F_S = \frac{Q_S \rho_S}{MW_S} \quad (3)$$

$$F_C = \frac{Q_F \rho_F x_C}{MW_C} \quad (4)$$

6.2 Effluent Gas Molar Flow Rate

The reformat effluent gas molar flow rate (F_R) on a dry basis at standard (T, P) conditions (0.0 °C, 760 mm Hg) is calculated by the next equation:

$$F_R = \frac{Q_R}{22,410} \quad (5)$$

6.3 Carbon Balance (C-Bal) and Nitrogen Balance (N-Bal)

The carbon and nitrogen balance parameter provides a relative indication of the accuracy of the measured test data. The greater the value deviates from 100 percent, the larger the experimental error is and the greater the molar balance uncertainty becomes. Carbon and nitrogen balances were calculated by analyzing the reactor effluent gas composition and flow rate after condensing out water vapor, and then applying the following formulas.

$$C - Bal = \frac{\text{mols Carbon Out}}{\text{mols Carbon In}} \times 100 = \frac{\left(\sum y_i \cdot n_i \right) F_R}{F_C \cdot \Omega_{GC}} \times 100 \quad (6)$$

$$N - Bal = \frac{\text{mols } N_2 \text{ Out}}{\text{mols } N_2 \text{ In}} \times 100 = \frac{y_{N_2} F_R}{0.79 F_A \cdot \Omega_{GC}} \times 100 \quad (7)$$

6.4 Hydrocarbon Conversion Efficiency (X_{HC})

The hydrocarbon conversion efficiency (X_{HC}) provides an indication of the relative quantity of “hydrocarbon slippage” in terms of CH_4 and any higher molecular weight (C_2^+) compounds exiting the monolith reactor. An X_{HC} value of 100 percent implies all carbon conversion in that no hydrocarbons were detectable in the reformer effluent. A reduced value of X_{HC} corresponds to a low carbon conversion into CO and CO_2 species. Hydrocarbon conversion efficiency was experimentally based on GC data measurements for hydrocarbons only in the reactor effluent gas and then calculated using the formula below.

$$X_{HC} = \left[1 - \frac{(y_{CH_4} + (\sum y_i \cdot n_i)) F_R}{F_C} \right] \times 100 \quad (8)$$

6.5 Space Velocity

The gas hourly space velocity ($GHSV$) is a term describing the number of reactor volumes of feed processed per hour per unit volume of catalyst. The higher the $GHSV$ performance is, the smaller the reactor volume becomes at a given volumetric throughput. The $GHSV$, which is referenced to standard state conditions (0.0 °C, 760 mmHg), has units of hr^{-1} and the same concept applies to the hydrocarbon liquid hourly space velocity ($LHSV$).

$$GHSV = \frac{(F_F + F_S + F_A)}{V_{cat}} \times 22,410 \quad (9)$$

$$LHSV = \frac{Q_F}{V_{cat}} \quad (10)$$

6.6 Steam to Carbon ($S:C$), Oxygen to Carbon ($O:C$) and Equivalence Ratio (ϕ)

The steam to carbon ratio ($S:C$) and oxygen to carbon ($O:C$) ratios are each based on the molar feed rates to the ATR. In the $O:C$ ratio definition, the basis used here is with respect to atomic oxygen fed to the reactor from the air stream only. The equivalence ratio (ϕ) is the inverse of the air stoichiometric mass ratio, and is defined as the actual mass ratio of fuel:air divided by the stoichiometric ratio, a term often used to describe combustion systems ($\phi \leq 1$) and partial oxidation conditions ($\phi > 1$).

$$S:C = \frac{F_S}{F_C} \quad (11)$$

$$O:C = 2. \times \frac{0.21 F_A}{F_C} \quad (12)$$

$$\phi = \frac{\left(\frac{F}{A}\right)_{actual}}{\left(\frac{F}{A}\right)_{Stoich}} = \left(\frac{A}{F}\right)_{Stoich} \left(\frac{W_F}{W_A}\right) = 14.62 \left(\frac{Q_F \rho_F}{Q_A \rho_A}\right) \quad (13)$$

where

F/A fuel-to-air mass ratio

(A/F)_{Stoich} stoichiometric air-to-fuel mass ratio (14.62 lb Air/lb Jet-A Fuel)

6.7 Reformer Efficiency (η_{Ref})

The reformer efficiency (η_{Ref}) is defined in terms of the lower heating value (LHV_i) of the hydrogen (H_2) and carbon monoxide (CO) products over the available chemical energy (LHV_F) of the Jet-A fuel feed as follows:

$$\eta_{Ref} = \left(\frac{(y_{H2} \cdot LHV_{H2} + y_{CO} \cdot LHV_{CO}) \cdot F_R}{Q_F \rho_F LHV_F} \right) \times 100 \quad (14)$$

where

LHV_{H2} 240.2 kJ/g-mol

LHV_{CO} 283.1 kJ/g-mol

LHV_F 43.435 kJ/g

6.8 Hydrogen Conversion Efficiency (X_{H2})

The hydrogen conversion efficiency (X_{H2}) expresses the ratio of the moles of H_2 in the product reformat gas to the moles of H_2 contained to the hydrocarbon fuel plus steam feed. Since the desired product from the reformer is gaseous H_2 , the X_{H2} parameter is a relative measure of the ATR catalysts' selectivity for forming hydrogen.

$$X_{H2} = \left[\frac{(y_{H2} \cdot F_R)}{\left(\frac{Q_F \rho_F x_H}{MW_{H2}} \right) + F_S} \right] \times 100 \quad (15)$$

It's noted that the hydrogen conversion efficiency does not take credit for the carbon monoxide present in the reformat. Carbon monoxide reacts with water to form hydrogen and CO_2 in the SOFC via the water gas shift reaction. For a PEM fuel cell system, the carbon monoxide is an anode material poison and must be removed from the reformat by a low temperature water-gas-shift reactor downstream of the reformer.

7. Results and Discussion

The reactor temperature profiles for each of the test catalysts screened are reported in figure 7. The data shows catalyst E-1 was operated at the lowest temperature of all catalysts tested. Sample E-1 was the only catalyst that was run at a constant 750 °C T_{fsp} while still maintaining a reformer efficiency above the 70 percent minimum. The next best monolith was the A-2 material, but it required a 20 °C temperature increase at 50 hr *TOS* in order to maintain its catalytic performance. In contrast, the least efficient catalyst sample B-6, required near continuous temperature adjustments, from initially 750 °C to a final temperature of 830 °C in order to offset its deactivation over time.

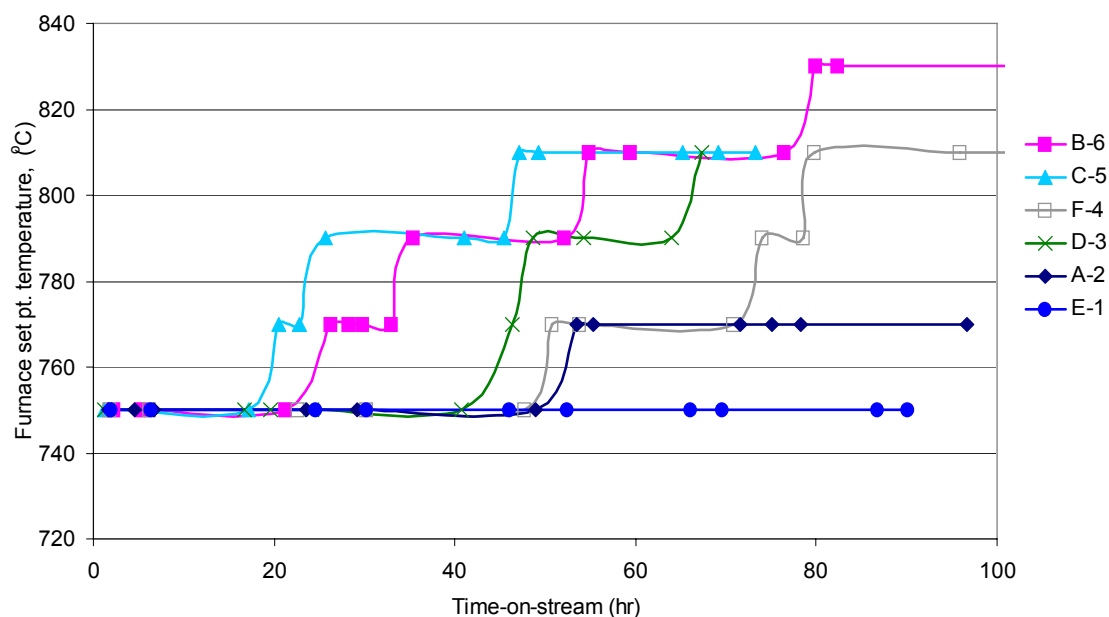


Figure 7.—Comparison of ATR reactor operating temperature (T_{isp})—all catalysts.

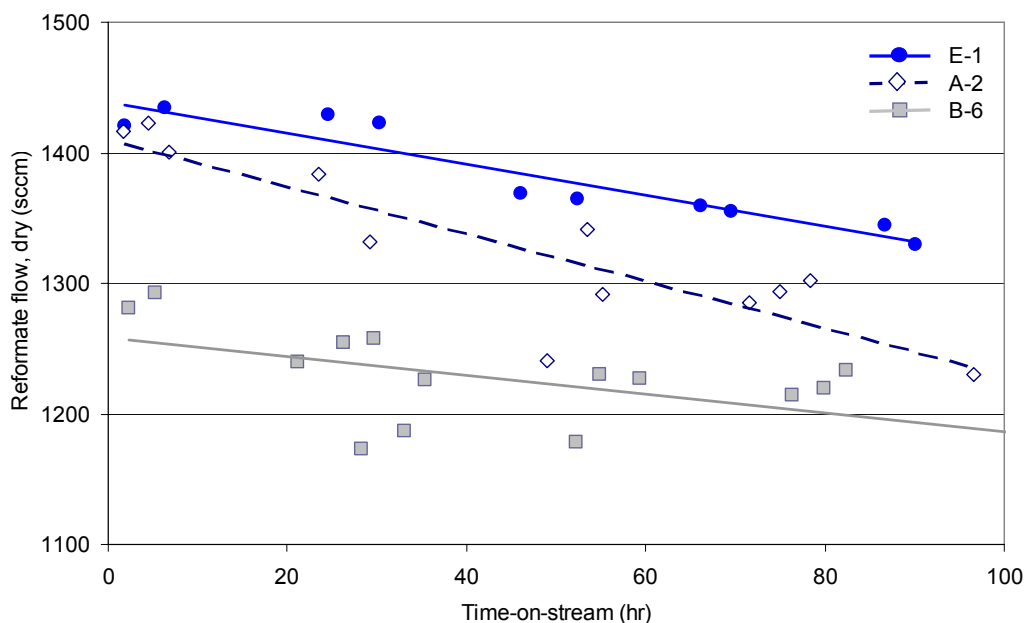


Figure 8.—Comparison of dry reformate flow rate (Q_R)—three catalysts.

The reformate gas flow rates, measured on a dry basis, for three of the six monolith samples tested is shown in figure 8. The highest reformate flow rate was generated with catalyst E-1 (1,383 sccm avg.) while B-6 had the lowest reformate flow (1,226 sccm avg.) measured exiting the ATR. The combined H_2 and CO molar flow rate data is given in figure 9. The $H_2 + CO$ flows ranged from an average high value of 1.81 g-mol/hr for catalyst E-1 to an average low value of 1.59 g-mol/hr for monolith B-6. The dry mole percent of the combined $H_2 + CO$ species found in the reformate gas was approximately 50 percent for all of the catalyst samples.

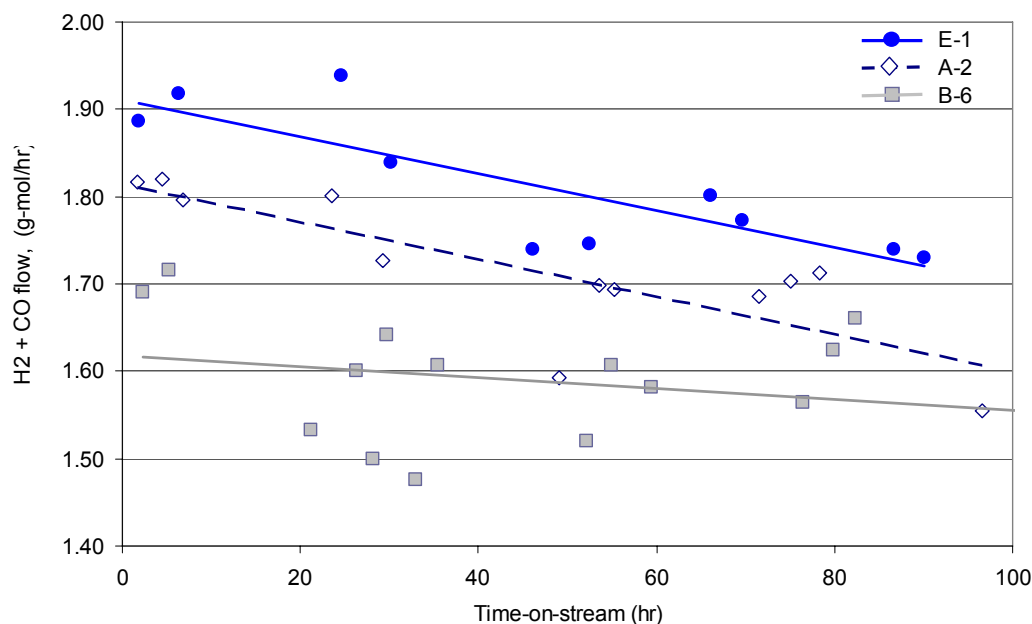


Figure 9.—Comparison of hydrogen and carbon monoxide molar flow—three catalysts.

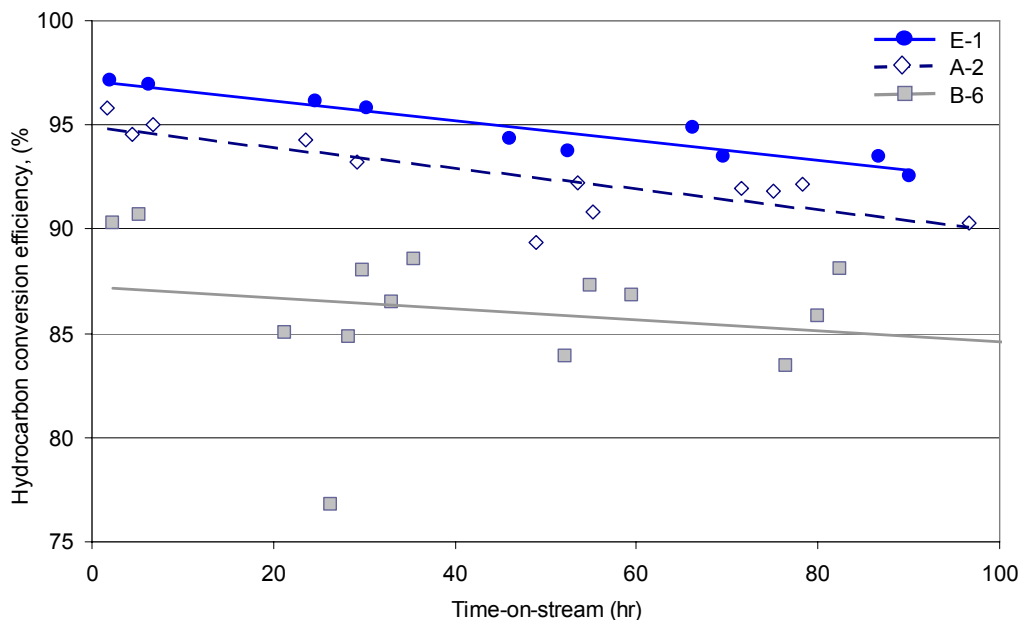


Figure 10.—Comparison of hydrocarbon conversion efficiency—three catalysts.

The hydrocarbon conversion efficiencies (X_{HC}) are reported in figure 10 for three of the six catalyst materials. The data shows the two highest performing catalysts, were E-1 and A-2, in comparison to the lowest performing material, the B-6 catalyst. Average values of X_{HC} ranged from 94.8 percent for E-1 to 86.0 percent for B-6. Catalyst sample A-2 was running about 2 percent less efficient than E-1 which had an average X_{HC} of 92.6 percent. The rate of change of X_{HC} over time for E-1 was 0.051 %/hr in comparison to 0.057 %/hr for A-2, thereby indicating a short-term reduction in catalyst activity for each of these monoliths.

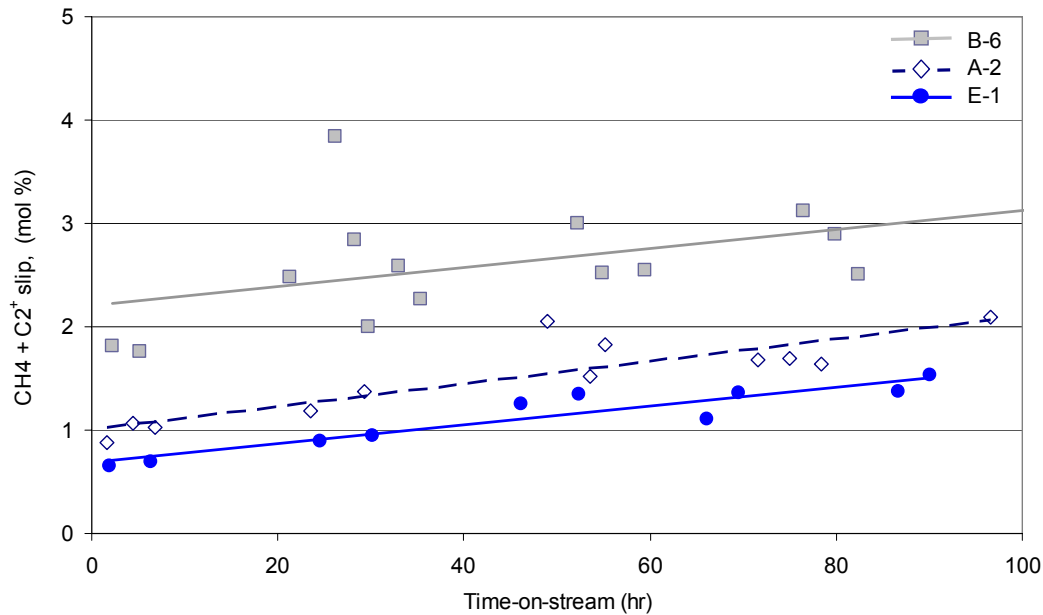


Figure 11.—Comparison of hydrocarbon slippage to reformat—three catalysts.

All of the catalysts tested in general showed a trend indicating increased hydrocarbon slippage as a function of *TOS*. Figure 11 provides a plot of the CH₄ and higher hydrocarbon (C₂⁺) mole percentages for the least active catalyst B-6 in comparison to the two highest performing catalysts E-1 and A-2. A hydrocarbon slippage of 1 percent or less is generally considered to be an acceptable value for virgin ATR catalysts with less than 1,000 hr *TOS*.

In SOFC hybrid applications, the reformer efficiency parameter (η_{Ref}), shown by the data in figure 12, is probably one of the best indicators of overall catalyst performance. The average reformer efficiencies for the six catalysts tested ranged from 75.4 to 83.4 percent. The two best catalysts were again found to be the E-1 and A-2 monoliths, with average reformer efficiencies of 83.4 and 80.2 percent, respectively. The least thermally efficient catalyst was the B-6 monolith which had an average η_{Ref} of 75.4 percent. The reformer efficiencies trends of the E-1 and A-2 catalysts both however showed decreases of 7.6 and 12.1 percentage points over the short duration test, respectively. The flatness of the reformer efficiency data for the B-6 catalyst was due to continuous temperature adjustments made during the experiment from 750 °C at *SOR* to 830 °C at *EOR*.

Figures 13 and 14 show the time-on-stream (*TOS*) performance of the E-1, A-2 and B-6 monoliths given in terms of two additional parameters: the hydrogen conversion efficiency (X_{H_2}); and, the ratio of hydrogen plus carbon monoxide to carbon dioxide, respectively. The average hydrogen conversion efficiency varied from a minimum of 25.2 percent to a maximum of 35.1 percent. Catalysts E-1 and A-2 were found to be the most selective catalysts in terms of converting hydrogen contained in the fuel and steam to the desired product of gaseous H₂.

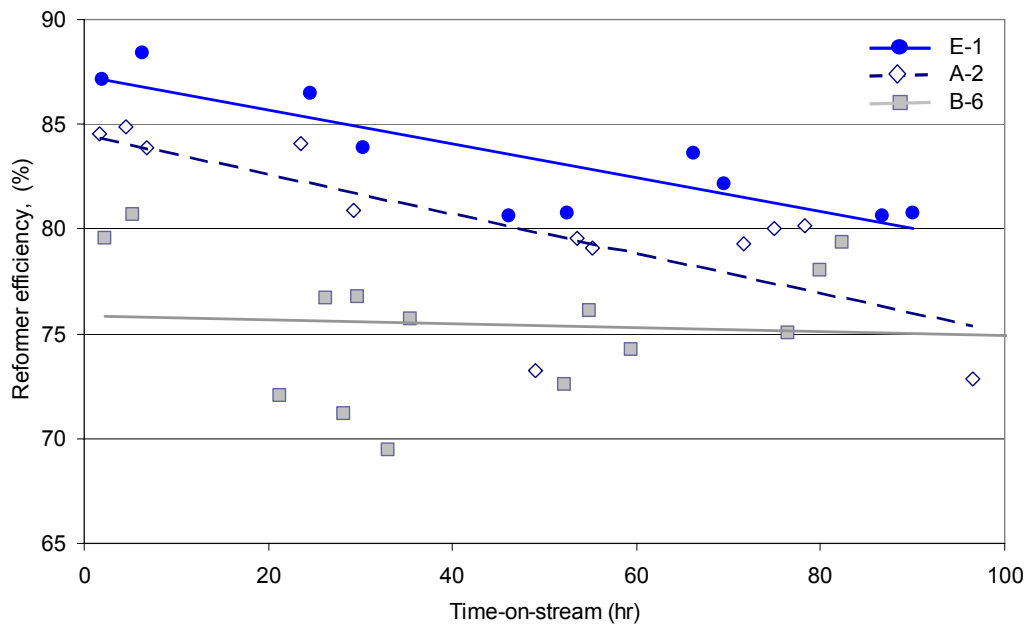


Figure 12.—Comparison of reformer efficiency—three catalysts.

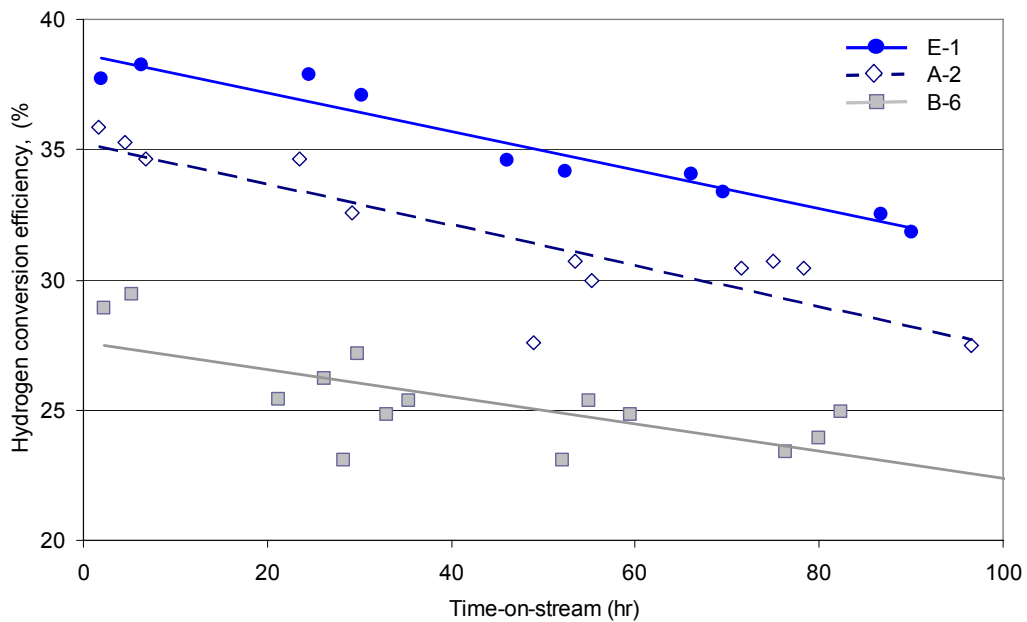


Figure 13.—Comparison of hydrogen conversion efficiency—three catalysts.

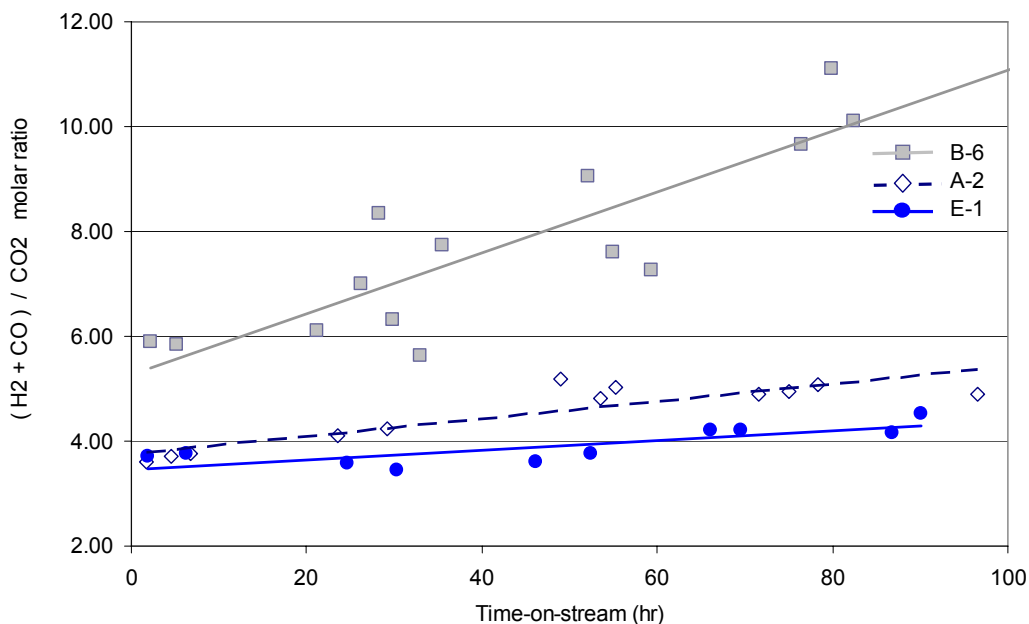
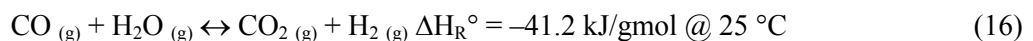


Figure 14.—Comparison of hydrogen and carbon monoxide to carbon dioxide ratio.

The figure 13 data further shows that the X_{H_2} of the two best performing catalysts, E-1 and A-2, decreased by 5.9 and 8.4 percent, respectively. The trend identified here during a short-term test indicates a deactivation rate of approximately 0.065 to 0.087 %/hr for each of the ATR catalysts. It's further observed that as the activity and selectivity of the catalytic materials apparently drop-off, the ratio of $(H_2+CO)/CO_2$ is increased as seen by the data in figure 14. This particular affect is thought to be attributed to the less active and selective catalyst forcing the water gas shift reaction, towards the right at a reduced rate, as indicated by the stoichiometry given below. In other words, for the case of the B-6 catalyst screening run, the $(H_2+CO)/CO_2$ ratio increases with time because both H_2 and CO_2 concentrations decline while CO concentration rises during the test.



To further study the affects noted above, thermodynamic equilibrium calculations (ref. 8) at 750°C were made with the E-1 catalyst reformat gas at start-of-run (*SOR*) and end-of-run (*EOR*) conditions. The experimental data is shown in table 6 and compared with the dry, N_2 -free equilibrium gas composition predictions. The analysis reveals that at *SOR*, the ATR achieved 96.0 percent of the equilibrium conversion to synthesis gas based on the concentration of H_2 as the reference.

At the *EOR* conditions, the test data indicates a significant decline from the equilibrium conversion to a lesser value of 90.2 percent. The difference between *SOR* and *EOR* equilibrium conversion for the E-1 catalyst represents a 6.1 percent reduction in performance with respect to initial catalyst conversion to H_2 . Since everything else was held constant during the screening test, this further verifies that a catalyst activity and selectivity reduction has occurred as previously suggested by the other test results and system parameters described before. The cause of the ATR catalyst deactivation is subject to further study and testing. Since these were only short duration screening tests, longer time on stream (*TOS*) runs would be needed to verify whether the catalyst deactivation rate either levels off as would be the case for a “break-in” period, or whether it continues along the trends found here. Figure 15 illustrates the overall performance test results of the E-1 catalyst on a single plot.

TABLE 6.—CATALYST E-1 REFORMATE GAS COMPOSITION COMPARED WITH EQUILIBRIUM PREDICTIONS.

Catalyst ID E-1	Start-of-Run (SOR) Dry, N ₂ -free gas, mol%		End-of-Run (EOR) Dry, N ₂ -free gas, mol%	
	Test	Predicted ¹	Test	Predicted ¹
Compound				
H ₂	62.7	65.3	58.9	65.3
CO	15.4	12.4	20.9	12.4
CO ₂	20.9	22.3	17.7	22.3
CH ₄	0.9	140 ppm	1.9	140 ppm
C ₂ ⁺	0.06	—	0.6	—
H ₂ equilibrium conversion, percent	96.0		90.2	

¹The equilibrium predictions were run at a S:C of 3.51, an O:C of 0.72 and a reaction temperature of 750 °C.

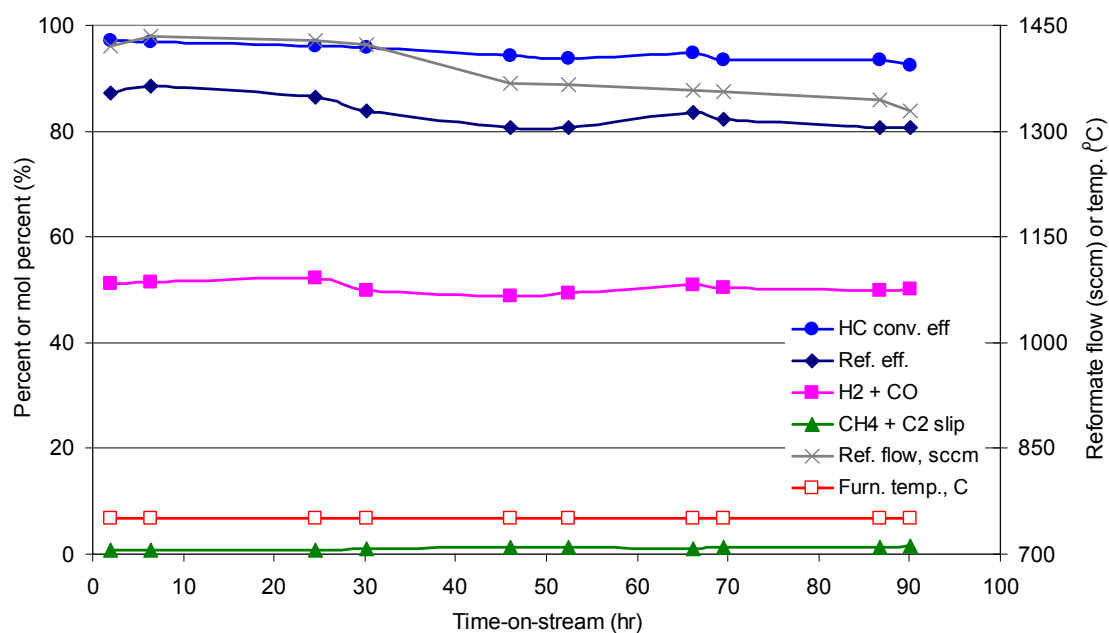


Figure 15.—Performance summary for catalyst E-1(S:C 3.5, O:C 0.72, GHSV 12,000 hr⁻¹).

7. Concluding Remarks

Six developmental autothermal reformer catalysts of monolith form were selected and tested in a 0.05 kW_e bench-scale micro-reactor. The hydrocarbon feed used was Jet-A fuel having a sulfur content of 1,500 ppm_w. The catalyst screening studies were carried out at the following reactor conditions: 750 to 830 °C, a GHSV of 12,014 hr⁻¹, a LHSV of 1.73 hr⁻¹, a S:C ratio of 3.51, and an O:C ratio of 0.72 (atomic oxygen). The only process variable changed during testing was the reactor furnace set point temperature that would be increased to compensate for catalyst deactivation. The choice of ATR process conditions

enabled meaningful catalyst performance differentiation in 70 to 100 hr of screening test time. Notable performance differences could be readily observed among the six candidate catalysts using this test protocol, thereby enabling rapid screening. The key test variables selected to rank catalyst performance in the order of their importance included the following:

- Reformer efficiency, η_{Ref}
- Hydrocarbon conversion efficiency, X_{HC}
- Hydrogen conversion efficiency, X_{H_2}
- Dry reformate flow rate, Q_R
- H_2 and CO generated, $F_{\text{H}_2} + F_{\text{CO}}$
- Low reactor furnace temperature, T_{fsp}

The best performing catalyst was found to be sample E-1. This monolith achieved the highest hydrocarbon conversion, and greatest reforming efficiency with highest H_2 concentration in the reformate gas at the lowest reactor temperature of 750 °C. In other words, catalyst E-1 was the most active and selective catalyst among the six candidate catalysts evaluated in the short-term screening tests. The second best performing monolith was determined to be catalyst A-2, although it required a 20 °C higher furnace temperature than E-1. The average reformer efficiencies for the two best performing catalysts, E-1 and A-2 ranged from 83.4 to 80.2 percent. Their corresponding hydrocarbon conversion efficiencies varied from 94.8 to 92.6 percent.

For all of the catalysts screened, the mole fraction on a dry basis of H_2 and CO product in the reformate gas was about 50 percent. All catalysts exhibited a trend showing decreased H_2 and CO_2 concentrations while the CO fraction increased versus *TOS*. Equilibrium conversion for the E-1 catalyst was analyzed and found to be 96.0 percent at *SOR* and 90.2 percent at *EOR* based on H_2 product concentration. All of the catalysts tested also showed a general trend towards declining activity and selectivity during the 100 hr test. Visual inspection of all tested catalysts did not indicate any carbon deposition, channel blockage or physical damage due to thermal sintering as a potential cause for loss of activity. Initial catalyst performance declines observed may be related to typical catalyst conditioning with real feed during start-up of the reactor. It's unknown whether any of these catalyst samples have been previously tested with a liquid hydrocarbon fuel by their suppliers.

Because the E-1 and A-2 monolith catalysts had the highest overall performance efficiencies, these materials were recommended and selected for further evaluation in a 1000 hr life-study test. Since the rate of catalyst deactivation has not been clearly established due to the limited *TOS*, a gas hourly space velocity of 6000 hr^{-1} for the life-study is proposed, using fresh monolith charges for both the E-1 and A-2 samples. The two best performing catalysts evaluated in the Phase I screening will be subsequently run through a 1000 hr durability test to characterize the long-term performance and catalyst deactivation rates during the Phase II portion of this program.

Appendix A

Catalyst Screening Test Data

Table I (cont.): Monolith catalyst screening test data – ATR with Jet-A.

Catalyst ID	TestID	TOS Total (hr)	Furnace Set T (°C)	Ref Exit T (°C)	N-Bal (%)	C-Bal (%)	HC-Conv Eff (%)	Ref Eff (%)	H2-Conv Eff (%)	Reformate Flow, dry (sccm)	Dry Reformate Composition (mol %)					
											H2	CH4	C2+	CO	CO2	N2
D-3	47	1.2	750	630	105.3	101.0	95.5	83.5	31.7	1347	37.1	0.9	0.14	14.9	10.2	36.7
		16.7	750	627	105.1	103.4	95.5	86.4	31.3	1336	36.7	0.8	0.18	16.8	8.9	36.6
		19.6	750	629	103.7	100.8	94.9	83.0	30.1	1302	36.2	1.0	0.19	16.6	8.9	37.1
		24.2	750	629	104.5	98.6	95.7	82.5	30.3	1308	36.4	0.8	0.16	16.2	9.0	37.4
		40.7	750	626	104.1	99.4	92.1	78.0	26.0	1226	33.0	1.3	0.42	19.0	6.9	39.3
		46.4	770	645	105.9	99.9	91.5	78.6	26.3	1247	33.0	1.6	0.35	18.8	6.7	39.5
		48.7	790	661	104.3	98.0	92.5	78.1	26.9	1254	33.9	1.6	0.23	17.8	7.5	39.0
		54.2	790	658	103.9	99.0	90.3	76.4	25.2	1223	32.4	1.9	0.44	19.1	6.5	39.7
		64.0	790	656	106.5	93.9	84.5	64.2	19.9	1109	27.8	2.5	1.12	18.9	5.4	44.2
	67.3	810	670	109.9	99.8	87.6	74.1	22.5	1200	29.3	2.3	0.63	20.8	4.5	42.5	
D-3	Avg.	38.3	770	643	105.3	99.4	92.0	78.5	27.0	1255	33.6	1.5	0.39	17.9	7.5	39.2
E-1	45	1.9	750	572	106.8	101.7	97.1	87.1	37.7	1421	41.0	0.6	0.04	10.1	13.7	34.5
		6.3	750	571	106.3	102.8	96.9	88.4	38.2	1434	41.3	0.6	0.05	10.2	13.7	34.1
		24.6	750	573	97.1	102.7	96.1	86.5	37.9	1429	42.3	0.8	0.06	9.9	14.6	32.3
		30.2	750	574	107.0	100.9	95.8	83.9	37.1	1423	40.7	0.9	0.07	9.1	14.5	34.8
		46.1	750	570	108.2	100.0	94.3	80.6	34.6	1368	38.9	1.1	0.16	10.0	13.6	36.2
		52.4	750	573	107.8	100.2	93.8	80.8	34.2	1365	38.7	1.1	0.20	10.5	13.1	36.3
		66.2	750	569	105.6	101.3	94.9	83.6	34.0	1359	38.8	0.9	0.18	12.2	12.1	35.8
		69.6	750	569	106.8	101.3	93.5	82.2	33.4	1355	38.2	1.1	0.26	12.2	11.9	36.3
		86.8	750	568	107.3	100.9	93.5	80.6	32.5	1344	37.6	1.1	0.26	12.3	12.0	36.8
	90.1	750	569	107.9	101.2	92.5	80.8	31.8	1330	37.0	1.2	0.35	13.1	11.1	37.3	
E-1	Avg.	47.4	750	571	106.1	101.3	94.8	83.4	35.1	1383	39.4	1.0	0.16	11.0	13.0	35.4
F-4	46	1.8	750	620	106.2	101.2	97.1	85.2	35.8	1398	39.4	0.7	0.03	11.0	13.1	34.7
		6.3	750	620	106.8	101.8	96.5	85.1	35.1	1396	38.7	0.8	0.05	11.6	12.5	35.0
		22.6	750	618	105.8	100.7	95.3	82.7	33.2	1349	37.8	1.0	0.10	12.6	11.7	35.8
		30.3	750	619	104.6	98.6	95.0	80.5	33.1	1340	38.0	1.1	0.11	11.6	12.3	35.7
		47.8	750	614	110.4	95.7	93.9	76.4	30.2	1315	35.3	1.2	0.18	12.4	10.9	38.4
		50.8	770	632	107.9	99.4	94.3	80.0	32.0	1340	36.7	1.2	0.10	12.4	11.5	36.8
		53.8	770	632	107.9	97.4	94.1	78.0	31.9	1342	36.6	1.3	0.11	11.3	12.0	36.8
		70.8	770	625	109.3	94.4	92.3	72.7	27.7	1264	33.6	1.5	0.28	13.4	10.0	39.5
		74.0	790	643	110.1	99.4	92.6	77.6	28.8	1305	34.0	1.5	0.23	14.5	9.6	38.5
	78.5	790	643	107.4	99.1	89.3	74.4	26.8	1252	32.9	1.8	0.55	15.4	8.7	39.2	
F-4	Avg.	79.8	810	658	106.8	100.4	93.1	79.4	31.4	1337	36.1	1.5	0.11	12.7	11.2	36.5
		95.8	810	653	107.3	98.5	89.2	73.3	24.6	1213	31.2	2.0	0.51	17.6	7.1	40.4
		100.1	810	654	107.8	97.0	84.5	66.6	21.6	1158	28.7	2.3	1.08	17.6	6.5	42.6
		102.8	810	652	108.0	96.6	83.5	65.1	20.8	1144	27.9	2.4	1.19	17.8	6.2	43.1

Appendix A Table I : Monolith catalyst screening test data – ATR with Jet-A.

Catalyst ID	TestID	TOS Total (hr)	Furnace Set T (°C)	Ref Exit T (°C)	N-Bal (%)	C-Bal (%)	HC-Conv Eff (%)	Ref Eff (%)	H2-Conv Eff (%)	Reformate Flow, dry (sccm)	Dry Reformate Composition (mol %)				
A-2	43	1.7	750	598	111.6	104.4	95.8	84.5	35.9	1416	H2	CH4	C2+	CO	CO2
		4.5	750	596	113.4	106.9	94.5	84.9	35.3	1423	38.9	0.8	0.11	10.5	13.7
		6.8	750	597	111.7	105.4	95.0	83.9	34.7	1400	38.1	0.9	0.20	11.1	13.3
		23.5	750	594	110.3	102.3	94.3	84.1	34.6	1383	38.0	0.9	0.16	11.4	13.1
		29.3	750	594	107.6	100.9	93.2	80.9	32.5	1332	38.5	1.0	0.20	11.6	12.2
		49.0	750	594	103.2	95.2	89.4	73.2	27.6	1241	37.6	1.1	0.31	12.4	11.8
		53.5	770	648	115.6	99.9	92.2	79.6	30.7	1341	35.1	1.2	0.81	14.4	9.5
		55.3	770	650	105.5	100.9	90.8	79.1	30.0	1292	35.4	1.1	0.41	13.4	10.1
		71.6	770	647	105.4	99.7	92.0	79.3	30.4	1286	36.0	1.3	0.39	14.1	10.3
		75.0	770	650	105.6	100.3	91.8	80.0	30.7	1294	36.4	1.3	0.39	14.1	10.3
		78.3	770	649	106.8	100.1	92.2	80.1	30.5	1302	36.6	1.3	0.41	14.1	10.2
		96.6	770	646	105.2	95.5	90.3	72.8	27.5	1230	36.2	1.3	0.37	14.4	10.0
		Avg.	760	622	108.5	101.0	92.6	80.2	31.7	1328	36.8	1.1	0.37	13.0	11.2
B-6	42	2.3	750	616	107.9	101.2	90.3	79.6	28.9	1281	34.9	1.1	0.69	15.9	8.6
		5.3	750	615	108.0	102.0	90.7	80.7	29.4	1292	35.2	1.1	0.62	15.9	8.7
		21.3	750	615	113.1	99.5	85.1	72.0	25.4	1240	31.8	1.4	1.13	15.8	7.8
		26.3	770	630	110.4	112.6	76.8	76.7	26.2	1254	32.0	1.5	2.32	17.2	7.0
		28.3	770	629	107.1	99.0	84.9	71.2	23.1	1173	30.5	1.5	1.36	18.7	5.9
		29.8	770	628	108.0	100.9	88.0	76.8	27.2	1258	33.7	1.3	0.72	16.5	8.0
		33.0	770	628	105.7	96.1	86.5	69.4	24.8	1186	32.4	1.5	1.12	15.5	8.5
		35.4	790	644	108.0	99.2	88.6	75.7	25.4	1226	32.2	1.5	0.74	18.2	6.5
		52.2	790	640	107.5	101.7	83.9	72.6	23.1	1178	30.2	1.7	1.30	19.4	5.5
		54.9	810	655	108.3	101.9	87.3	76.1	25.4	1230	31.9	1.7	0.80	18.4	6.6
		59.4	810	653	108.2	100.9	86.8	74.3	24.8	1227	31.6	1.8	0.77	18.0	6.8
		76.4	810	653	111.8	105.5	83.4	75.0	23.4	1215	29.7	1.9	1.26	19.9	5.1
		79.9	830	670	109.9	105.7	85.8	78.0	23.9	1220	30.2	2.0	0.94	21.0	4.6
		82.4	830	668	109.1	104.4	88.1	79.4	25.0	1234	31.2	1.8	0.69	20.6	5.1
		100.9	830	668	109.0	103.4	84.1	73.6	22.2	1169	29.0	2.0	1.17	21.0	4.4
		Avg.	789	641	108.8	102.3	86.0	75.4	25.2	1226	31.8	1.6	1.04	18.1	6.6
C-5	44	1.2	750	639	105.9	97.6	92.0	76.7	30.4	1306	36.6	1.1	0.50	12.7	11.3
		17.2	750	631	103.7	96.6	89.4	73.5	26.3	1201	33.8	1.2	0.83	16.0	8.5
		20.5	770	648	105.3	98.9	91.0	77.0	28.2	1254	34.8	1.3	0.55	15.5	9.1
		22.8	770	648	106.4	99.6	89.8	76.4	27.8	1253	34.3	1.4	0.67	15.6	8.9
		25.7	790	664	105.6	100.6	90.6	78.6	28.7	1270	35.0	1.4	0.52	15.8	8.9
		41.1	790	661	105.0	99.5	90.0	76.4	27.6	1241	34.3	1.5	0.59	16.0	8.8
		45.4	790	662	106.4	99.4	89.8	76.4	26.6	1237	33.4	1.5	0.64	17.1	7.8
		47.1	810	678	106.2	101.3	90.4	79.0	27.8	1268	34.1	1.5	0.51	17.0	8.0
		49.3	810	678	106.1	100.4	91.4	78.8	28.2	1274	34.5	1.5	0.40	16.5	8.5
		65.3	810	677	106.9	101.2	90.0	77.9	27.3	1269	33.7	1.6	0.52	16.9	8.1
		69.2	810	677	108.2	101.4	89.8	77.6	27.3	1266	33.5	1.7	0.53	16.7	8.2
		73.3	810	676	107.1	101.5	87.5	75.7	25.6	1230	32.3	1.8	0.82	17.9	7.1
		Avg.	788	662	106.1	99.8	90.2	77.0	27.6	1256	34.2	1.5	0.59	16.1	8.6
		39.8													39.0

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13. ABSTRACT (Maximum 200 words) Solid oxide fuel cell systems used in the aerospace or commercial aviation environment require a compact, light-weight and highly durable catalytic fuel processor. The fuel processing method considered here is an autothermal reforming (ATR) step. The ATR converts Jet-A fuel by a reaction with steam and air forming hydrogen (H ₂) and carbon monoxide (CO) to be used for production of electrical power in the fuel cell. This paper addresses the first phase of an experimental catalyst screening study, looking at the relative effectiveness of several monolith catalyst types when operating with untreated Jet-A fuel. Six monolith catalyst materials were selected for preliminary evaluation and experimental bench-scale screening in a small 0.05 kW _e micro-reactor test apparatus. These tests were conducted to assess relative catalyst performance under atmospheric pressure ATR conditions and processing Jet-A fuel at a steam-to-carbon ratio of 3.5, a value higher than anticipated to be run in an optimized system. The average reformer efficiencies for the six catalysts tested ranged from 75 to 83 percent at a constant gas-hourly space velocity of 12,000 hr ⁻¹ . The corresponding hydrocarbon conversion efficiency varied from 86 to 95 percent during experiments run at reaction temperatures between 750 to 830 °C. Based on the results of the short-duration 100 hr tests reported herein, two of the highest performing catalysts were selected for further evaluation in a follow-on 1000 hr life durability study in Phase II.				
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